

# Reologie is overal (part 2)

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University of Technology

**Where innovation starts**

## three cases

- case 1: brain tissue (biomechanics)
- case 2: carnivorous plant (biology)
- case 3: semi-crystalline polymers (polymer physics)

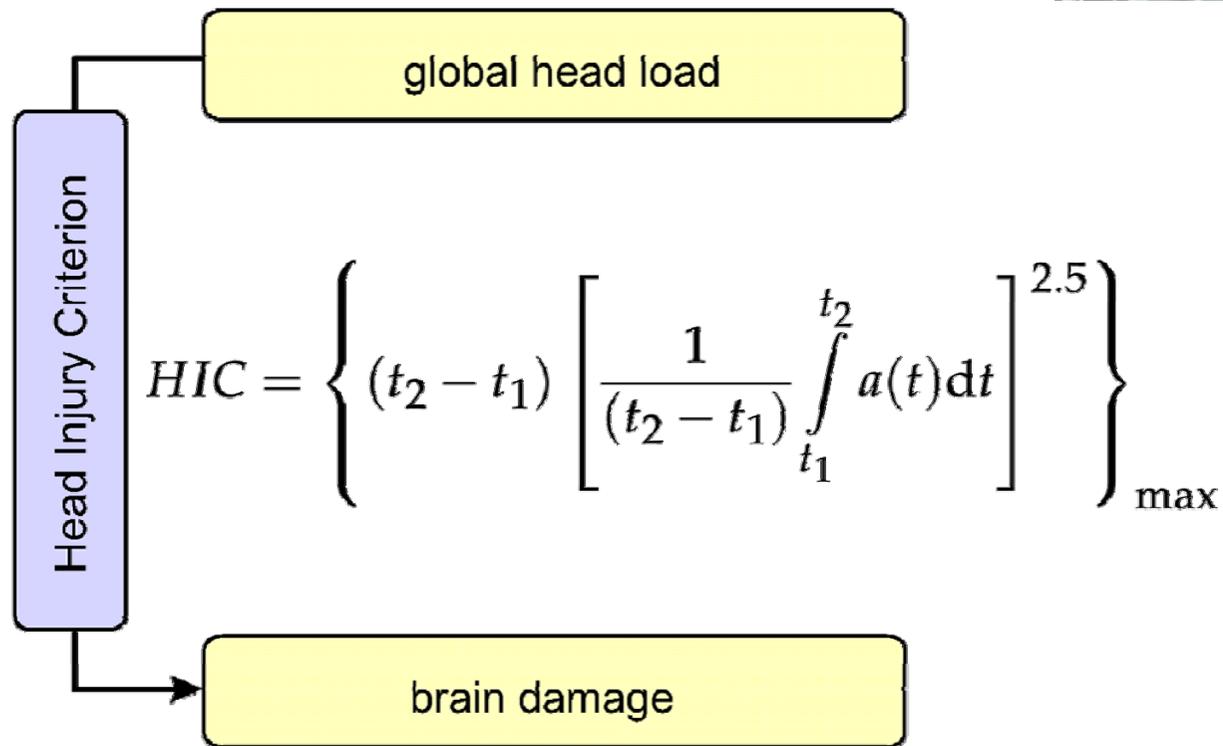
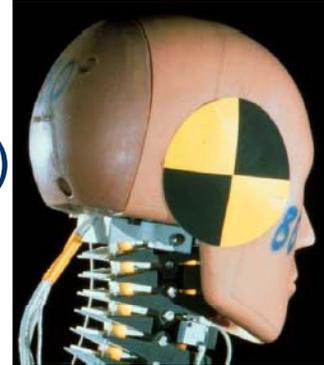
## introduction: traumatic brain injury

- large deformation (strain) → Traumatic Brain Injury (TBI)
- often occur during rotational and translational acceleration of the head
- exact mechanism of TBI still incompletely understood



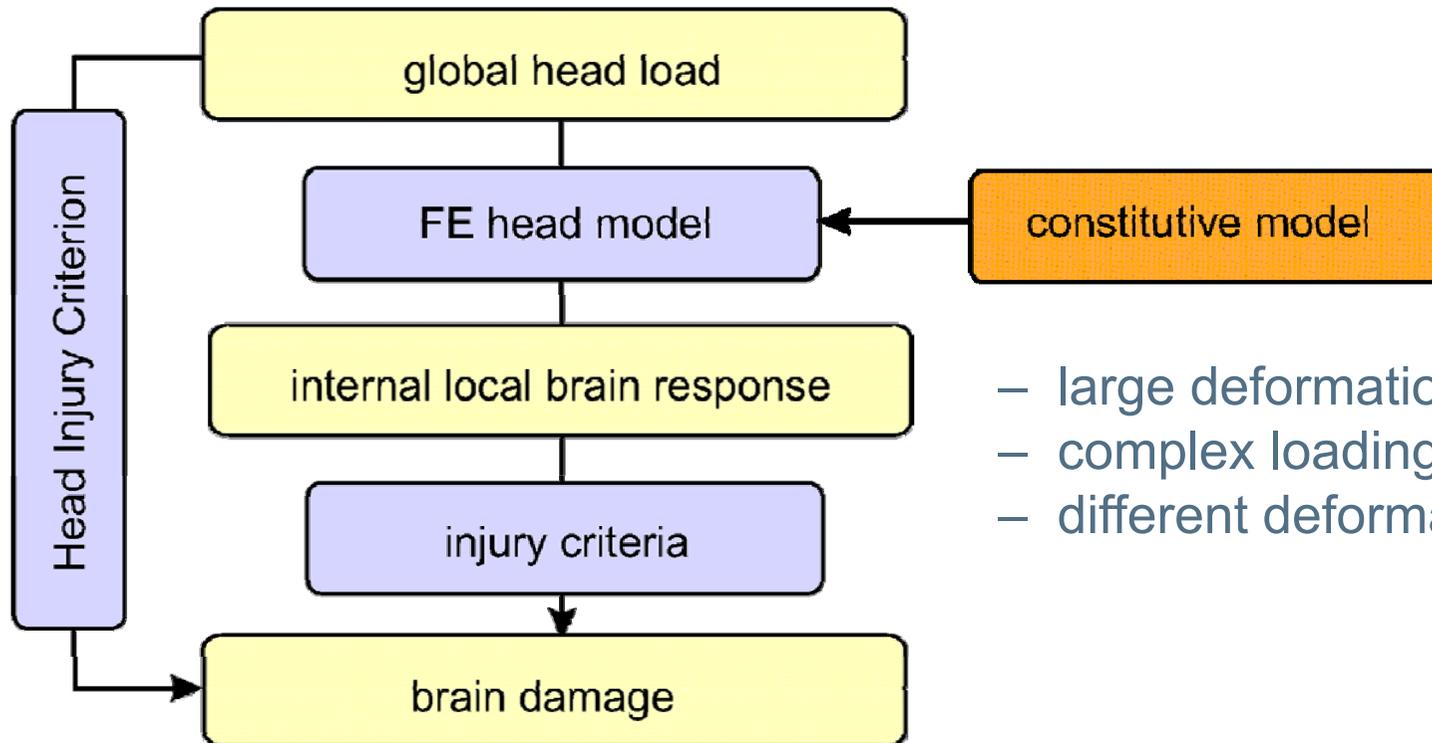
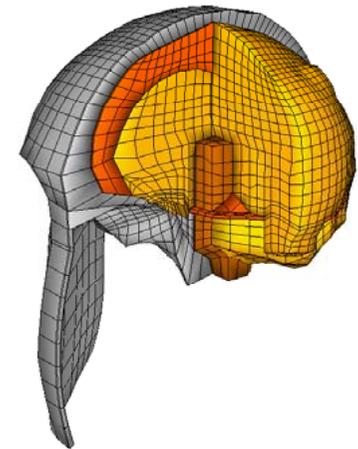
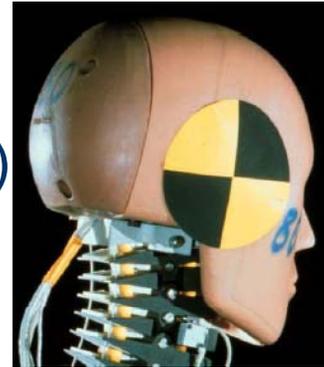
# introduction: traumatic brain injury

- Injury assessment (industry):
  - anthropomorphic test devices (ATD)
  - Head Injury Criterion (HIC)



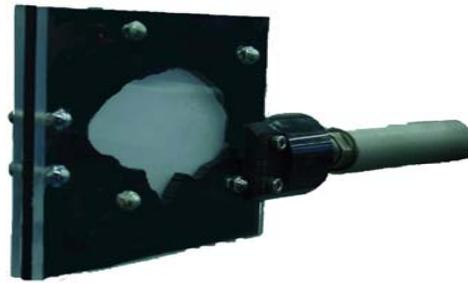
# introduction: traumatic brain injury

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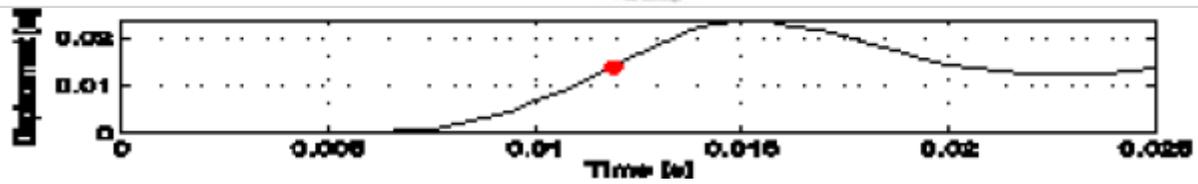
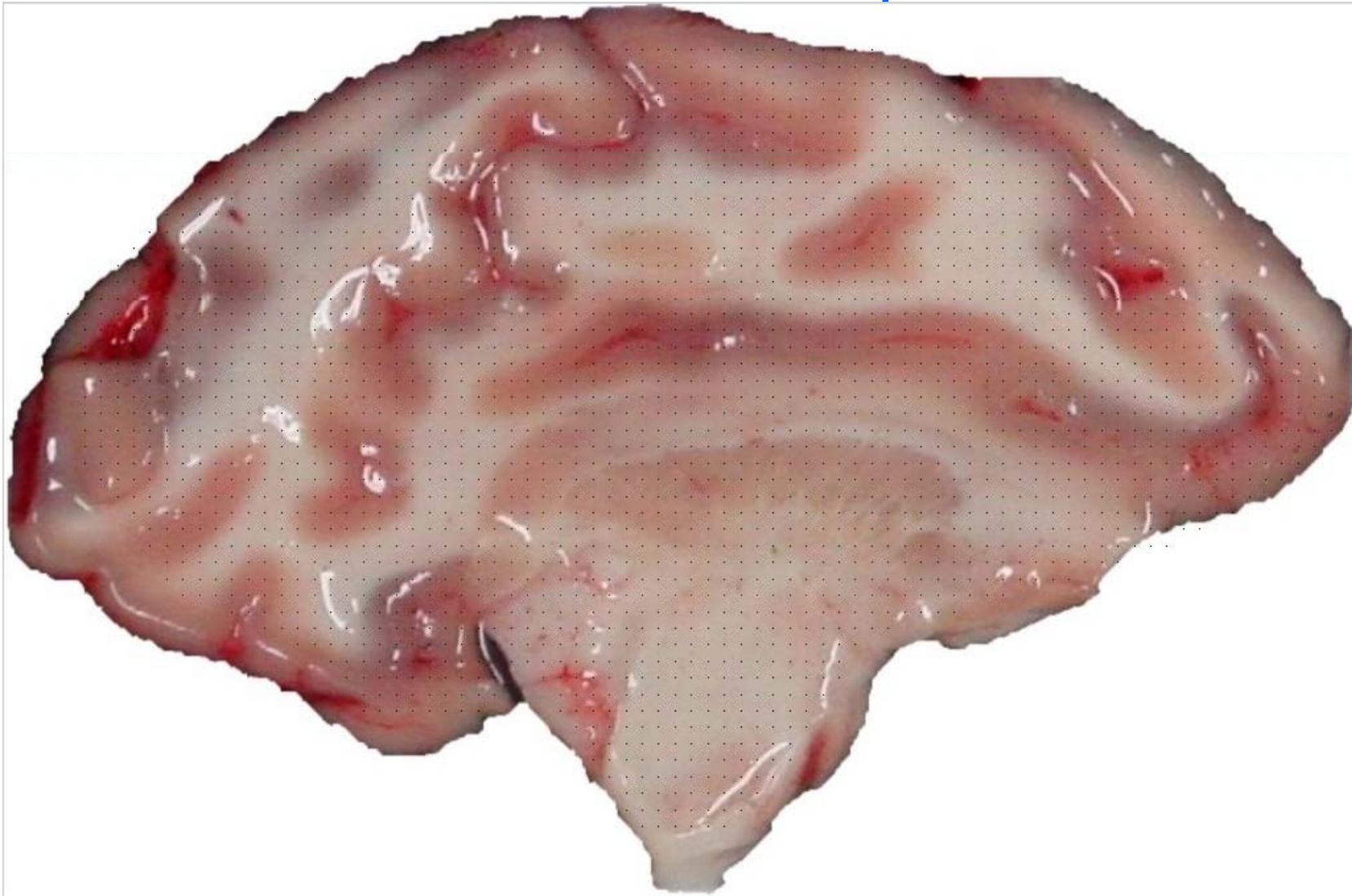
- large deformations
- complex loading paths
- different deformation modes

# brain deformations: experiment

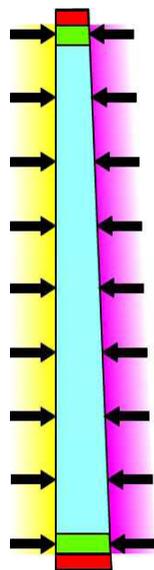
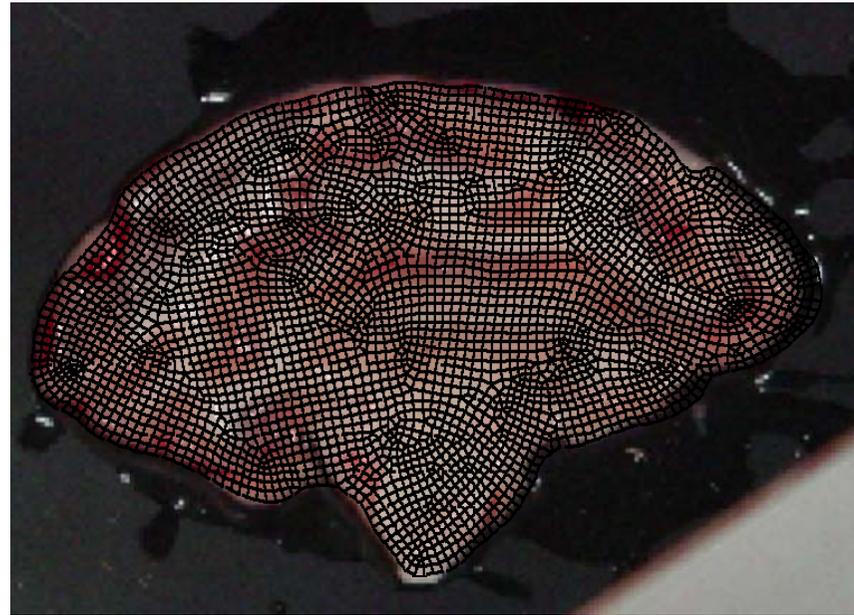


test device (high speed loading)

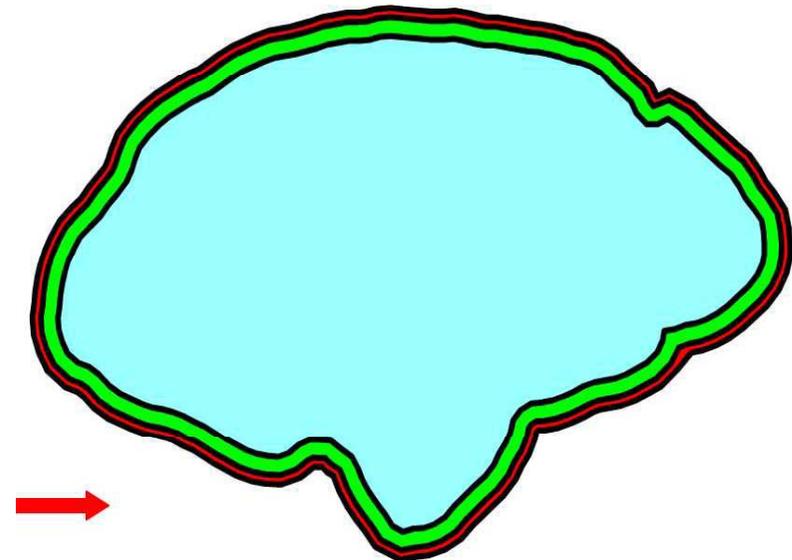
# brain deformations: experiment



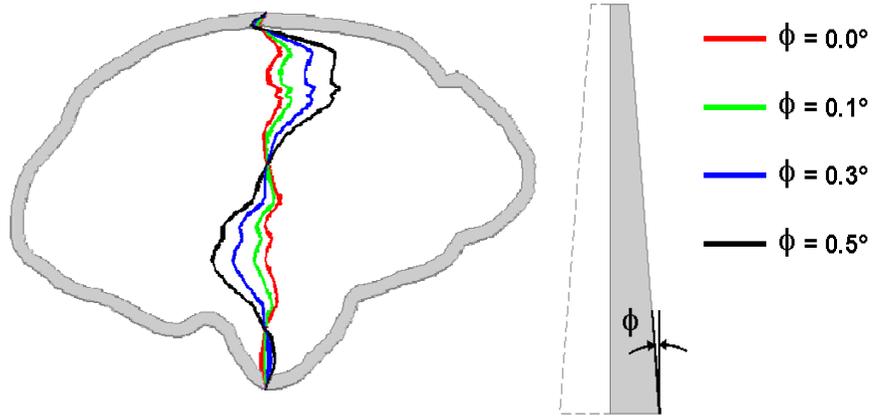
# brain deformations: experiment / simulations



- Skull
- aCSF
- Brain

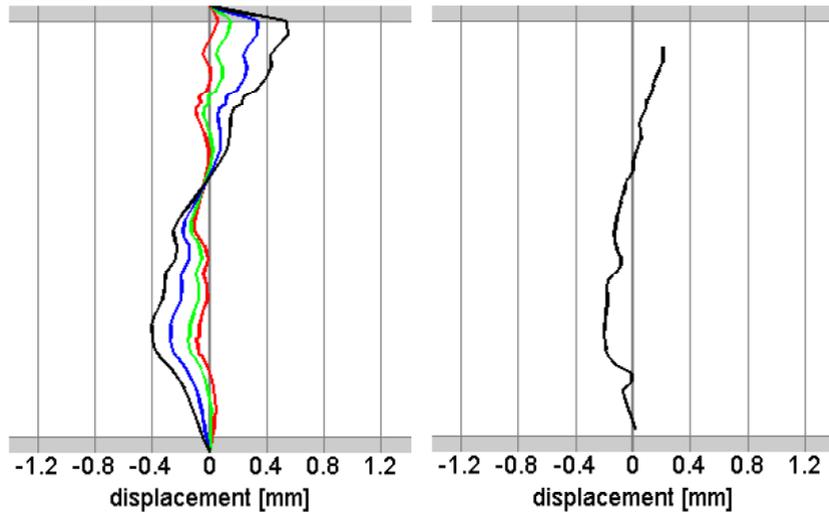


# brain deformations: experiment / simulations



Simulations

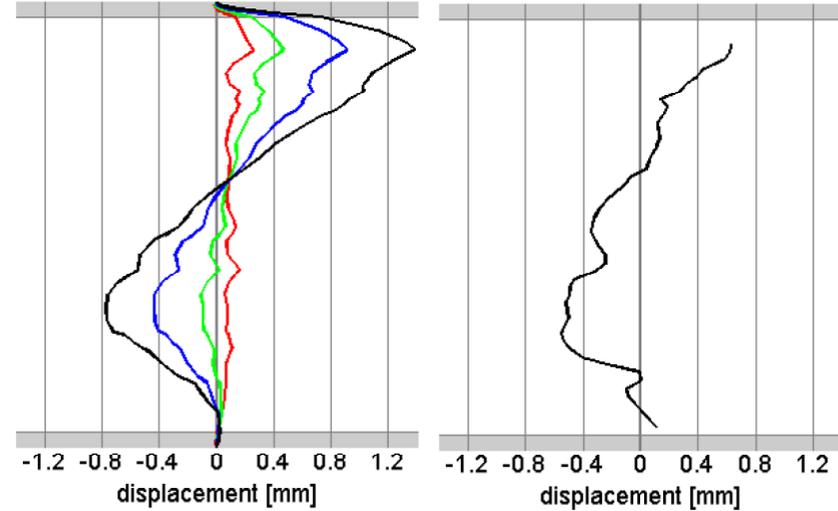
Experiment



$t = 8$  ms

Simulations

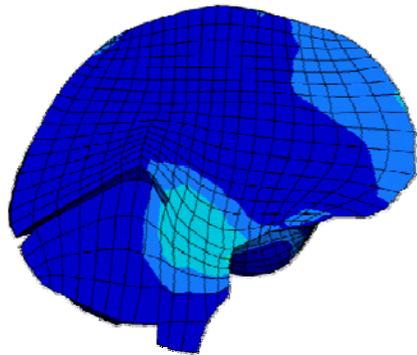
Experiment



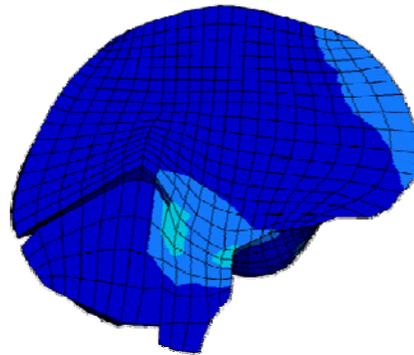
$t = 12$  ms

# model application

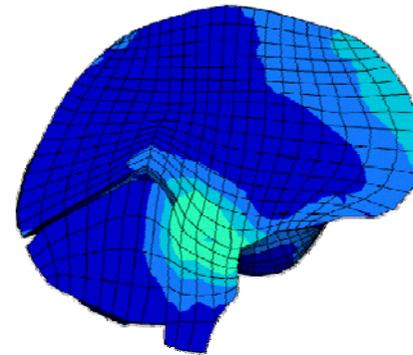
Current model



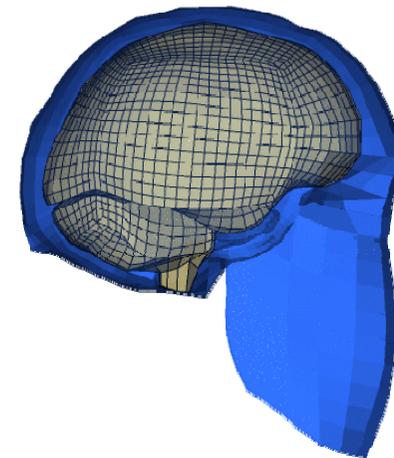
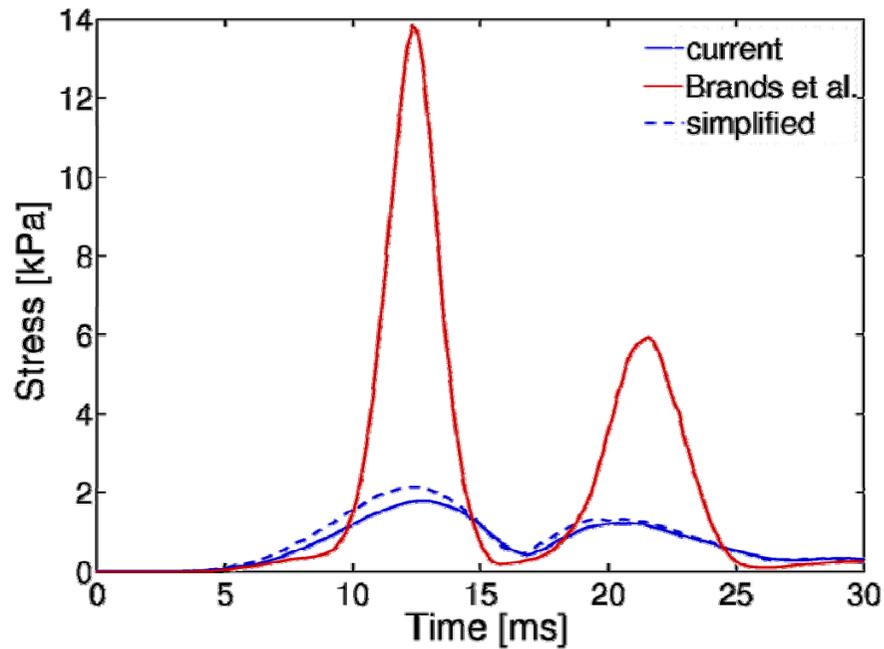
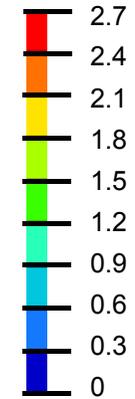
Brands et al. model



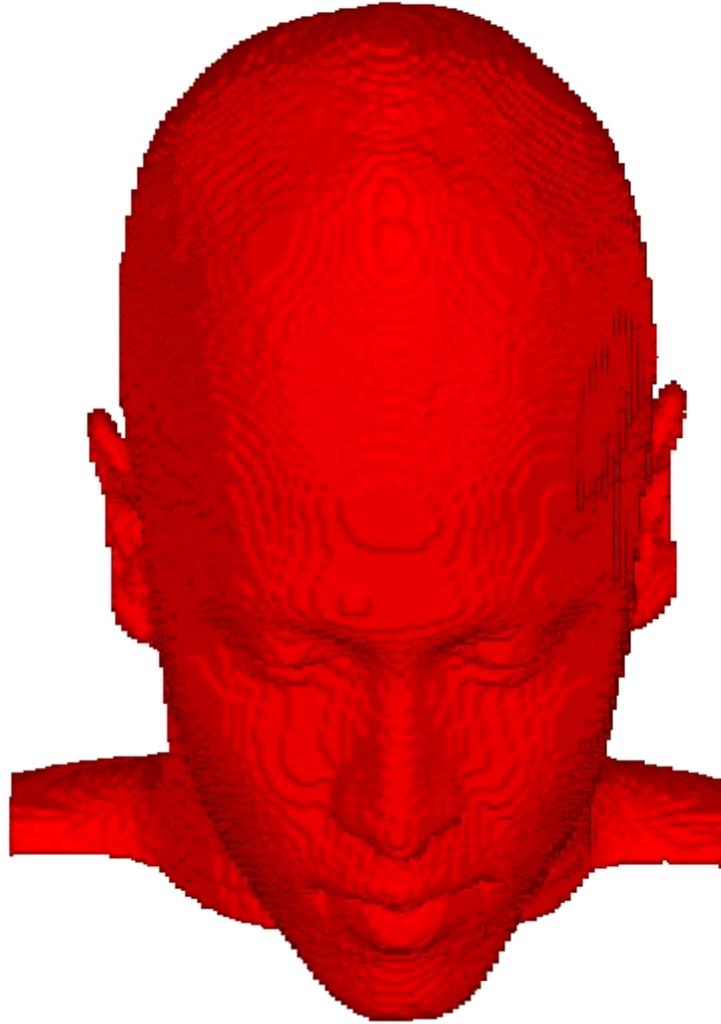
Current model simplified



Stress [kPa]



# model application

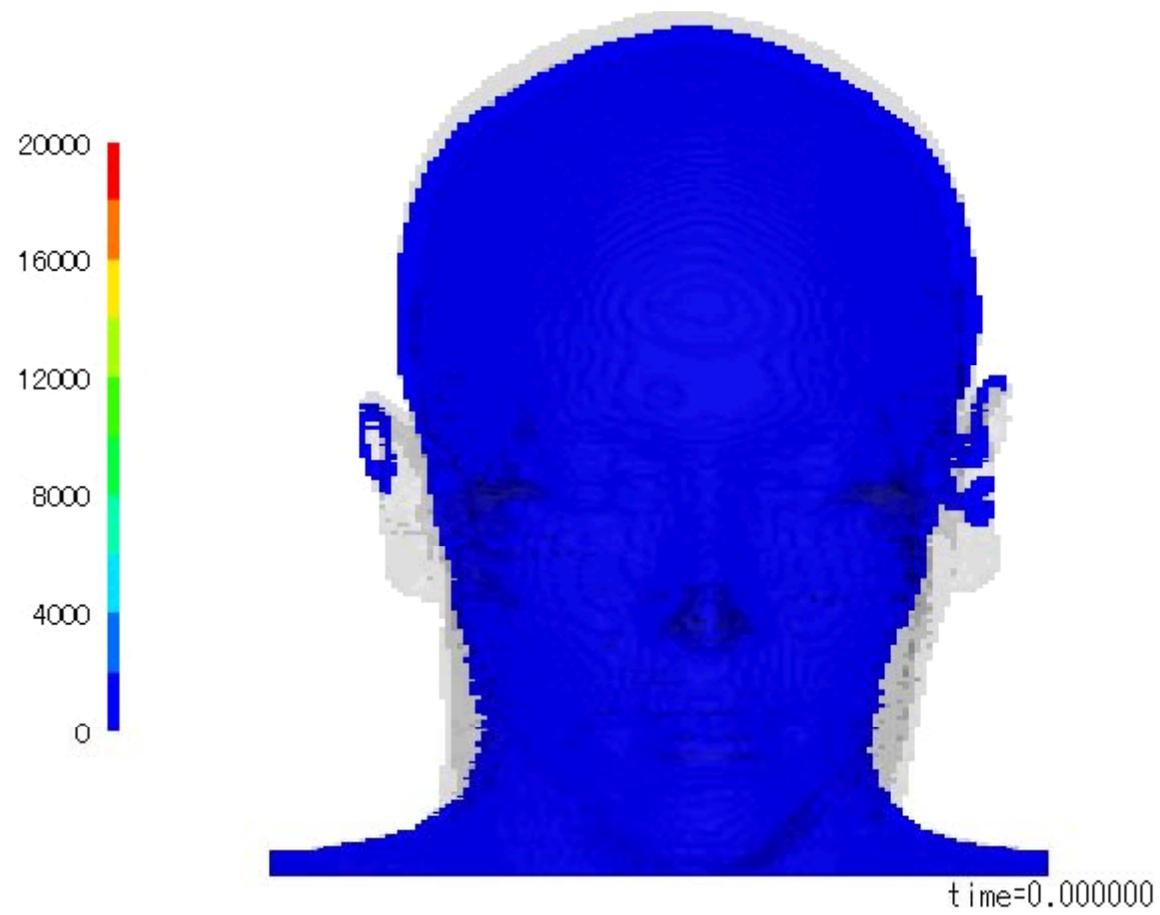


# model application



time=0.000000

# model application



# brain deformations: protection design



## three cases

- case 1: brain tissue (biomechanics)
- case 2: carnivorous plant (biology)
- case 3: semi-crystalline polymers (polymer physics)

# viscoelastic deadly fluid in carnivorous plants

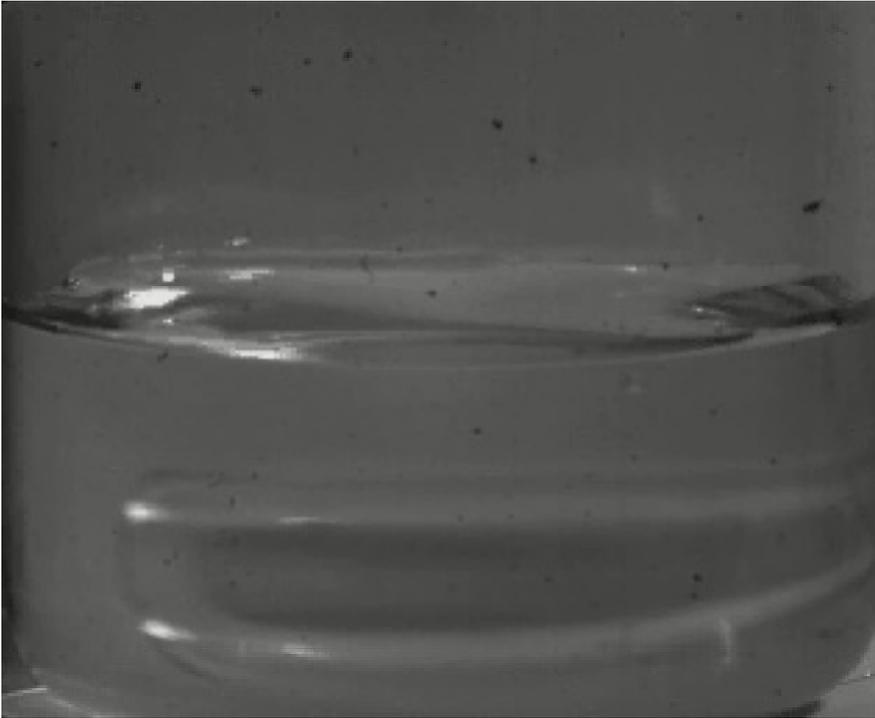
Laurence Gaume (Montpellier) & Yoel Forterre (Marseille)

the *Nepenthes rafflesiana*.



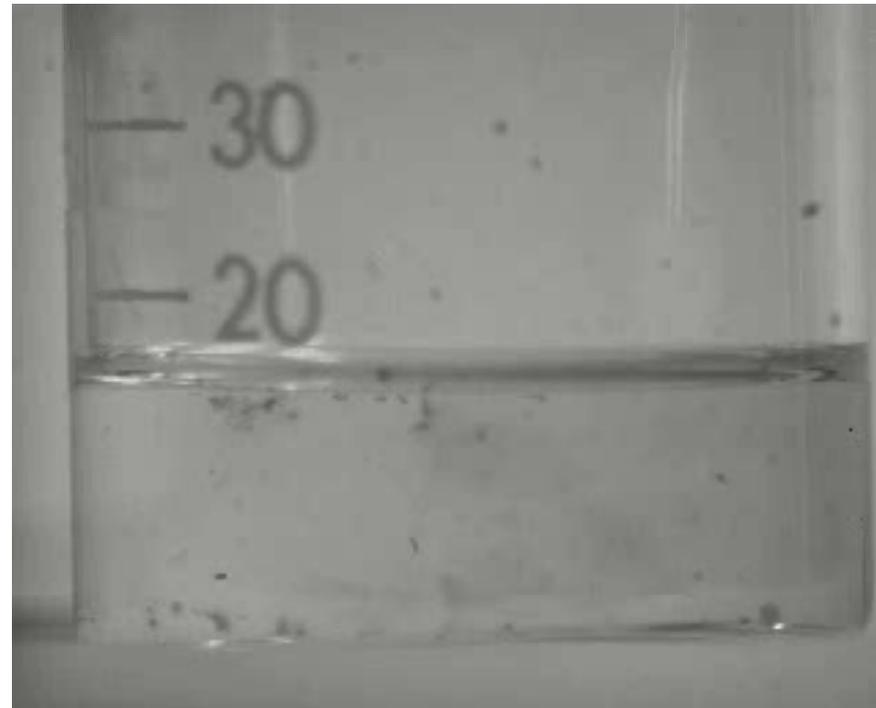
- Contains a fluid composed of water and polysaccharides

# a fly tries to flee

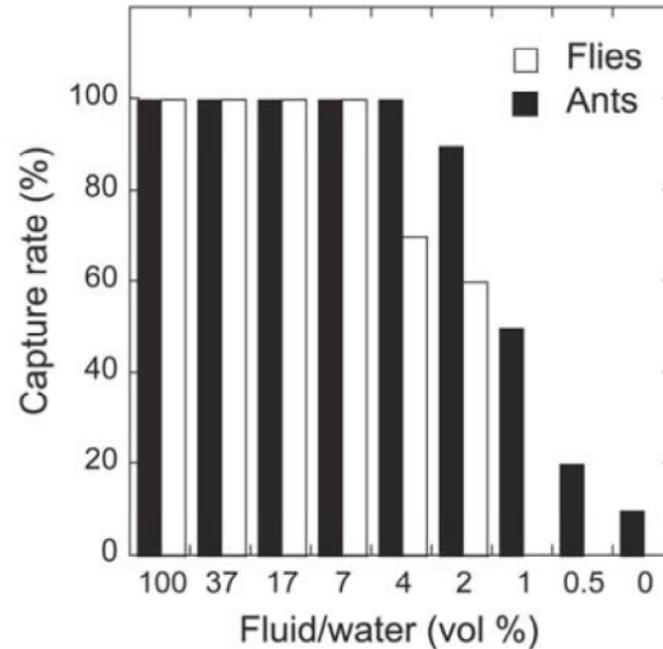


water

fluid

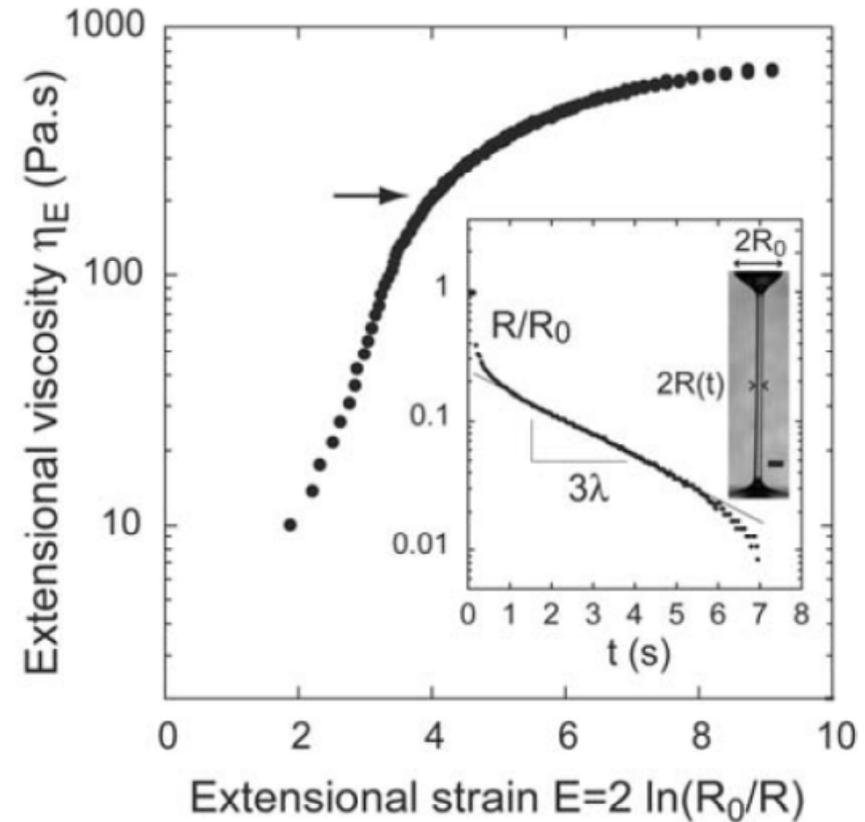
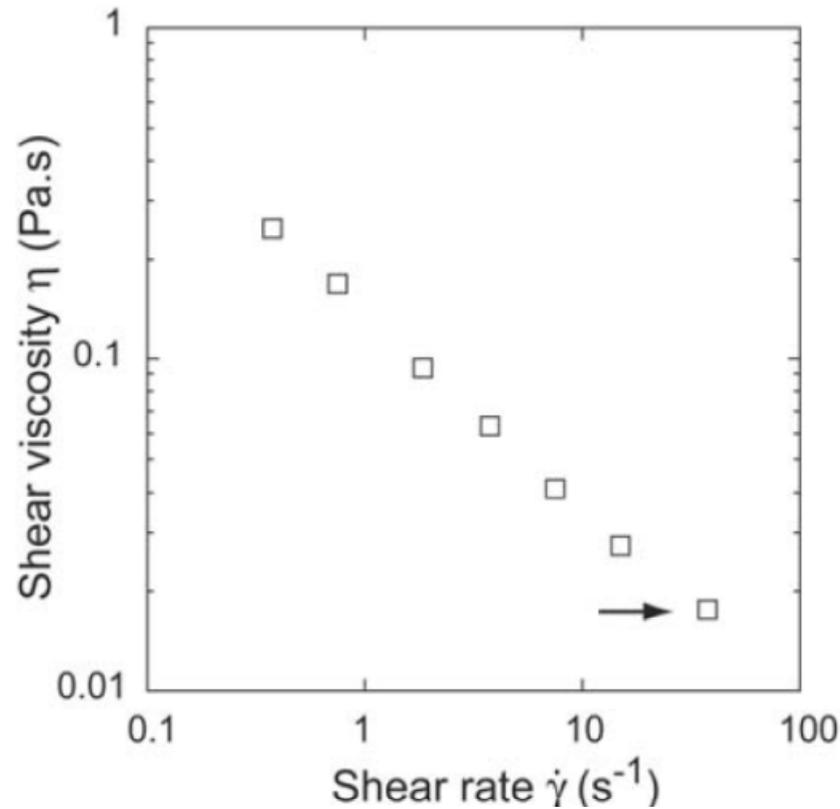


# influence of concentration



- it's not a chemical attack (insects recover when removed from the fluid)
- surface tension hardly varies with concentration: surface tension doesn't explain ( $\sigma_{\text{fluid}} = 0.0726 \text{ N.m}$ ,  $\sigma_{\text{water}} = 0.0720 \text{ N.m}$ ).

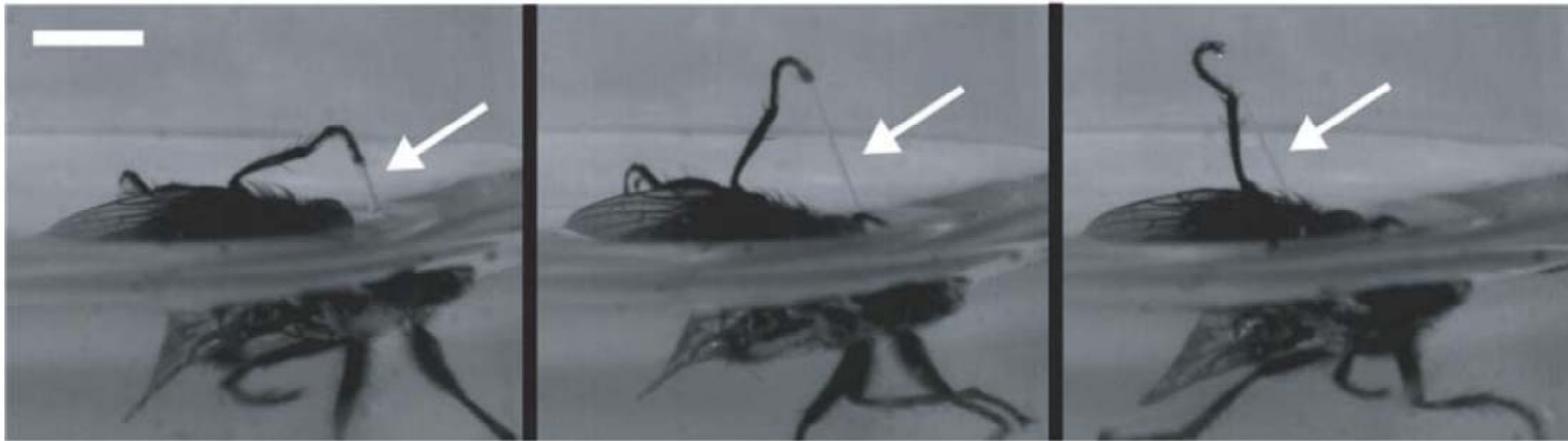
# drag forces: viscosities of the pure fluid



shear viscosity /shear rate (left)    transient extensional viscosity / strain (right)

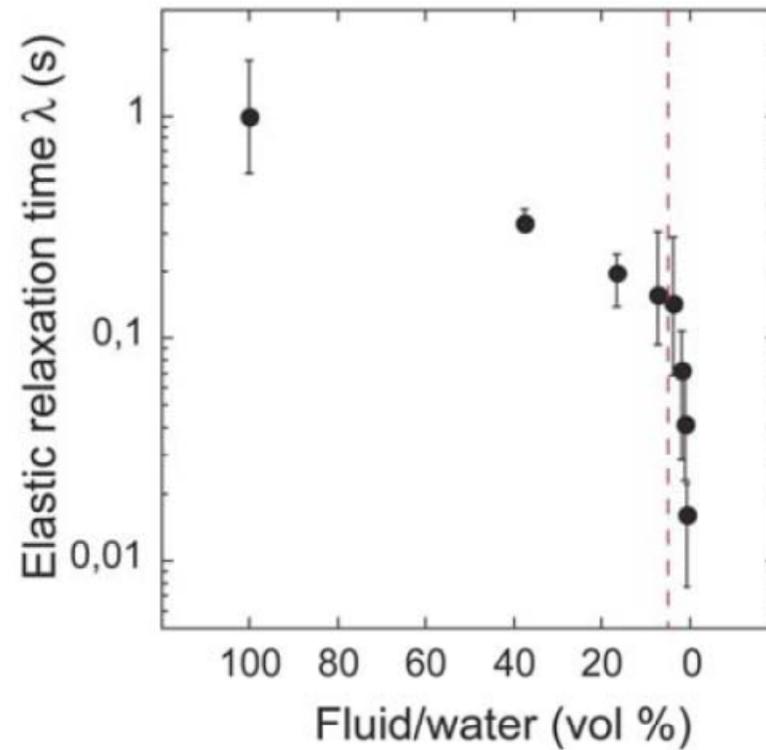
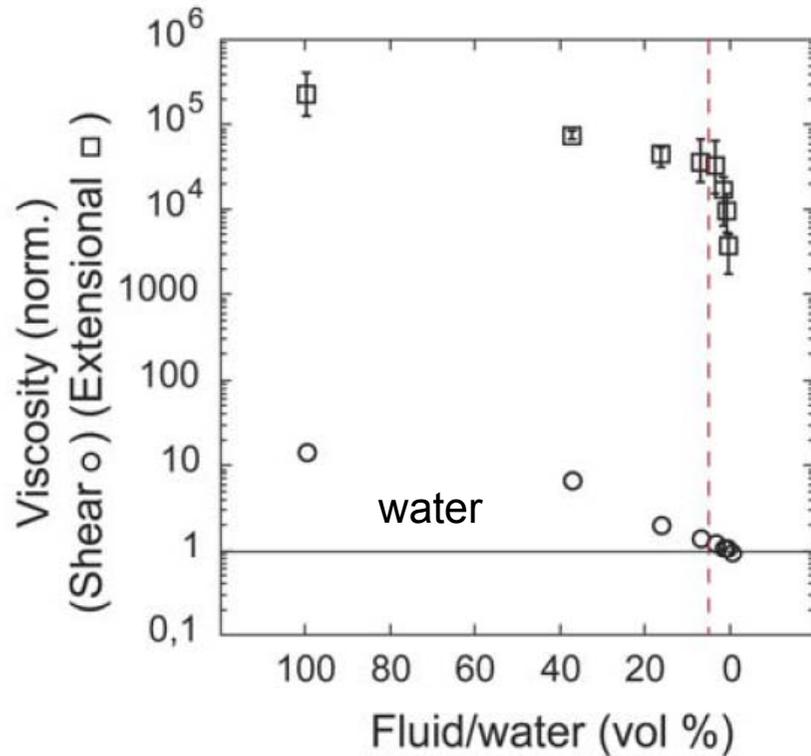
arrows indicate typical values corresponding to insect motion in the fluid

## elongational effects: filament formation



dynamical sequence of a fly in the digestive fluid showing a viscoelastic liquid filament attached to its leg (arrows)

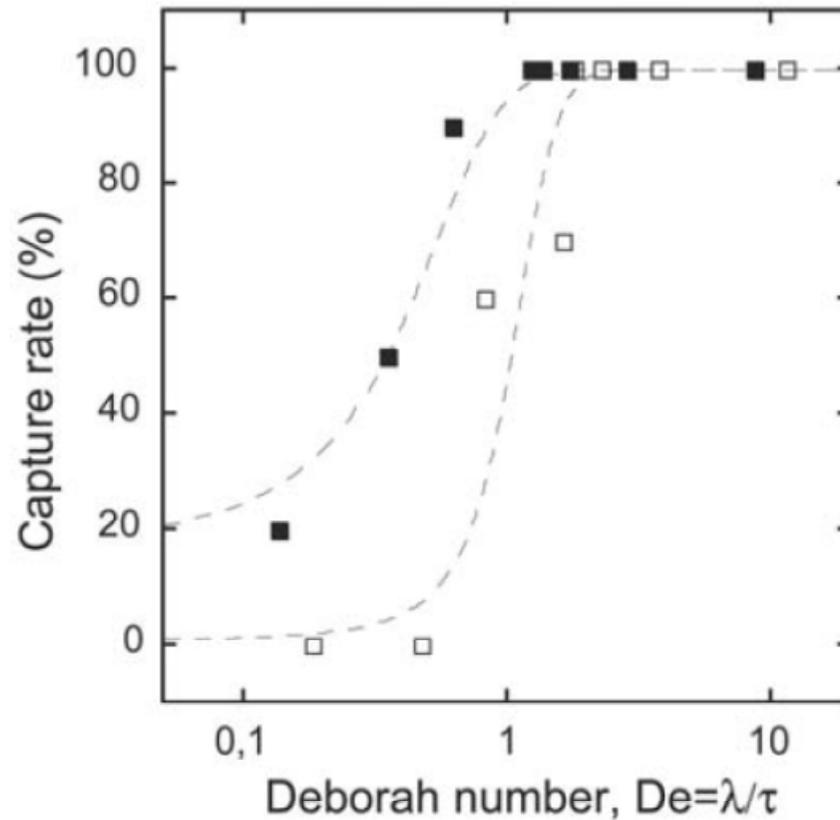
# viscosities: influence of concentration



dilution effect on the shear ( $\circ$ ) and extensional viscosity ( $\square$ ) (left)

dilution effect on the characteristic relaxation time (right)

# capture rate versus De-number



-trapping efficiency is conditioned by both fluid viscoelasticity and insect dynamics

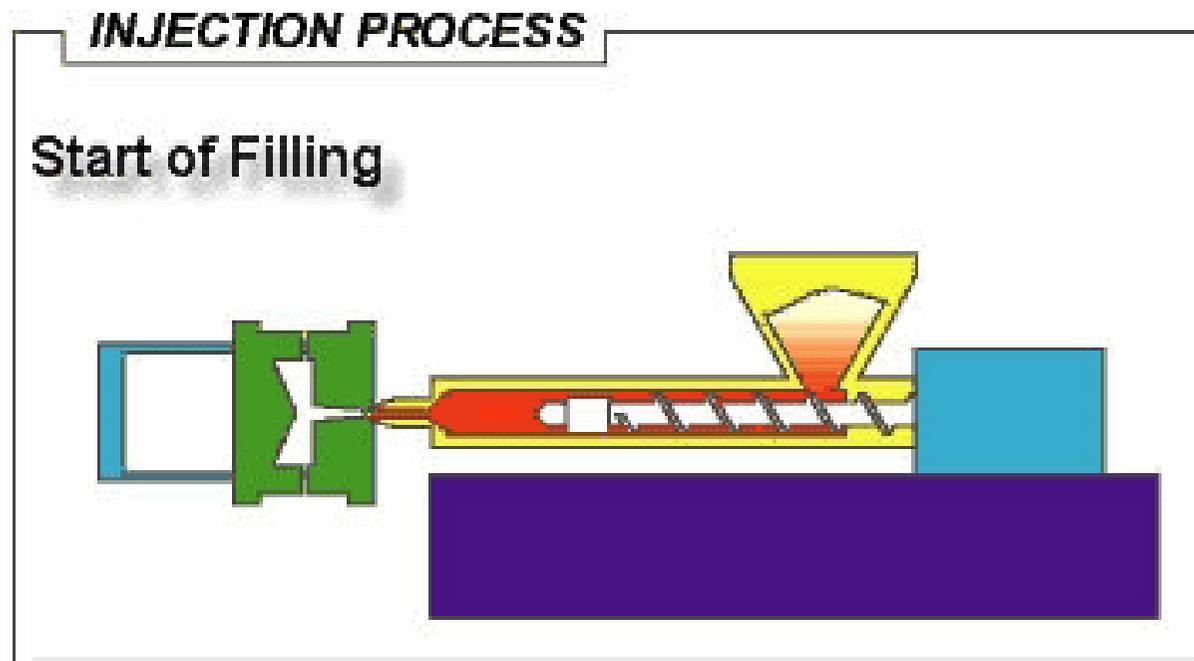
- tropical plants, often submitted to high rainfalls and thus variations in fluid concentration.

capture rate / Deborah number (flies □, ants ■)

## three cases

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- case 3: semi-crystalline polymers (polymer physics)

# injection molding



# load-bearing applications of polymers

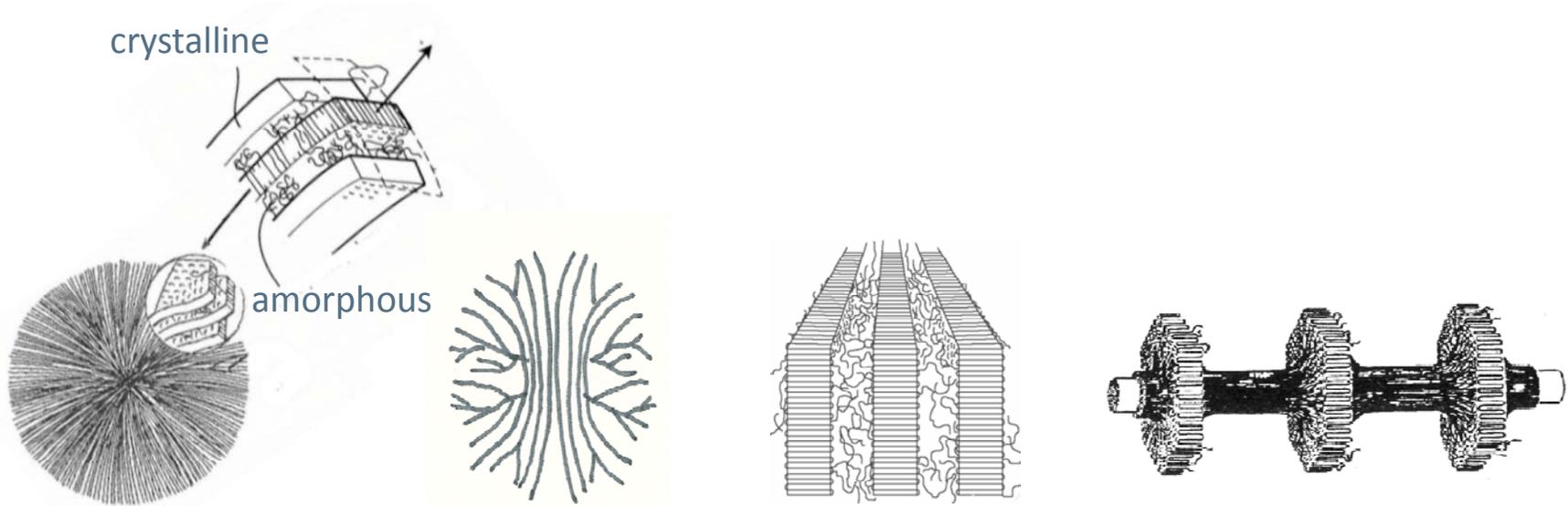


# processing of semi-crystalline polymers



- Polymer processing:  
high  $\dot{\gamma}$ , high  $p$  and high  $\dot{T}$   $\rightarrow$  structure formation
- Mechanical behaviour:
  - Influence of morphology

# structure development during flow

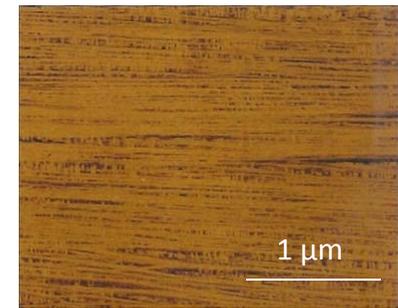
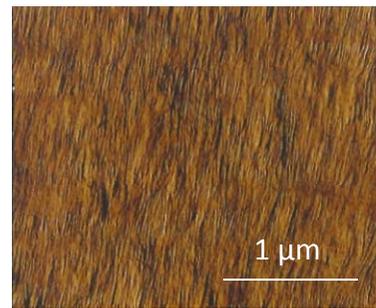
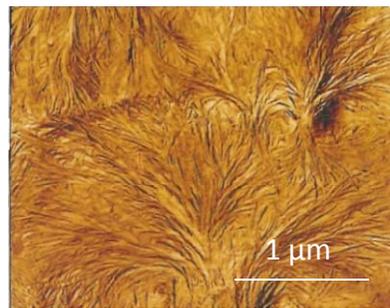
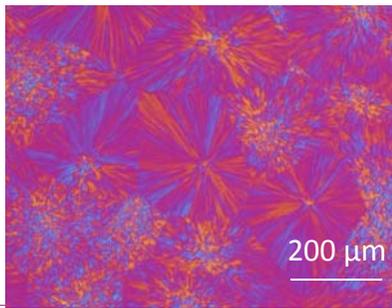


isotropic spherulites

slightly oriented spherulites

row structure

shish kebab



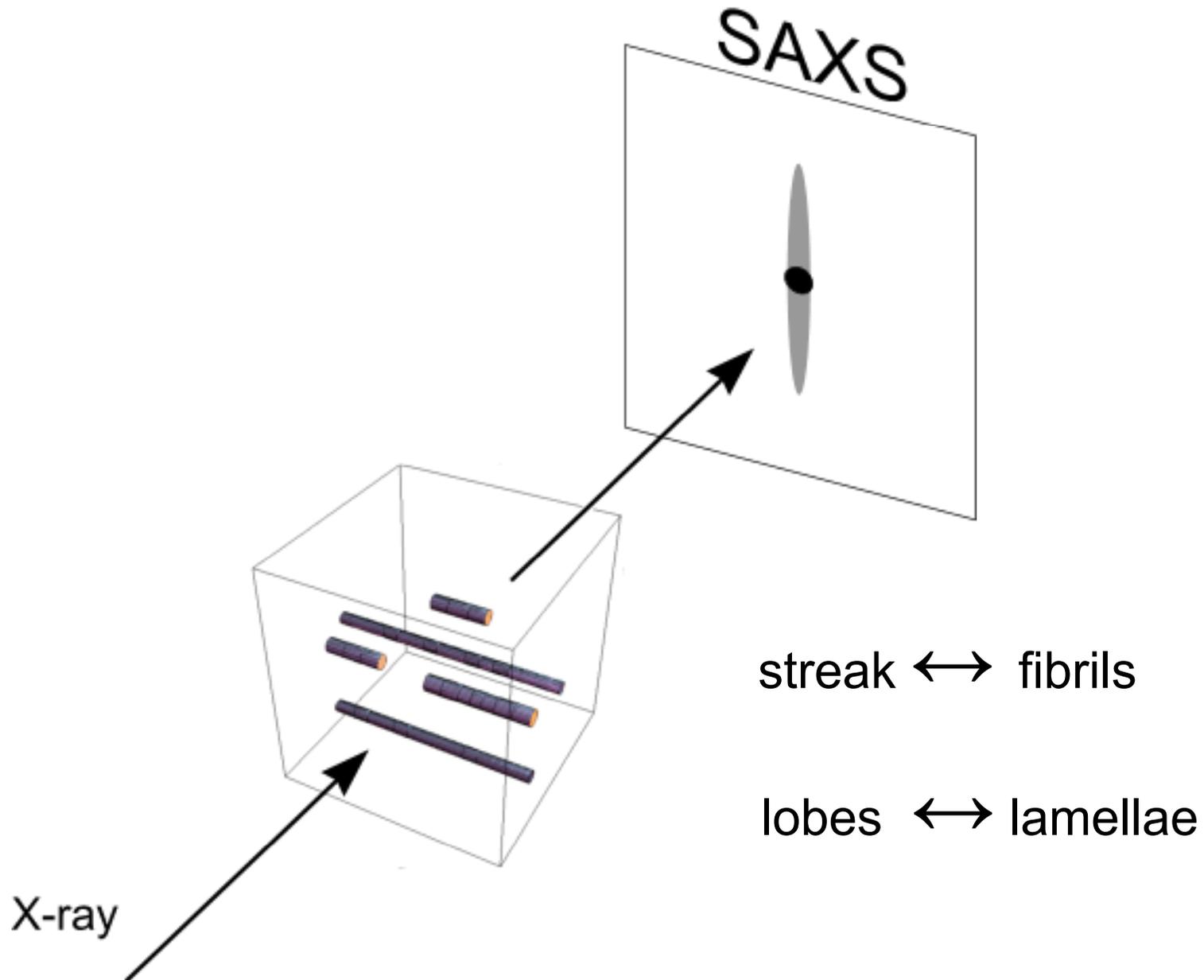
no orientation

flow

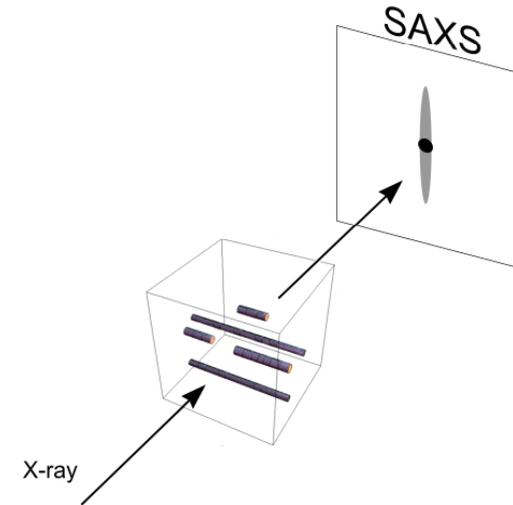
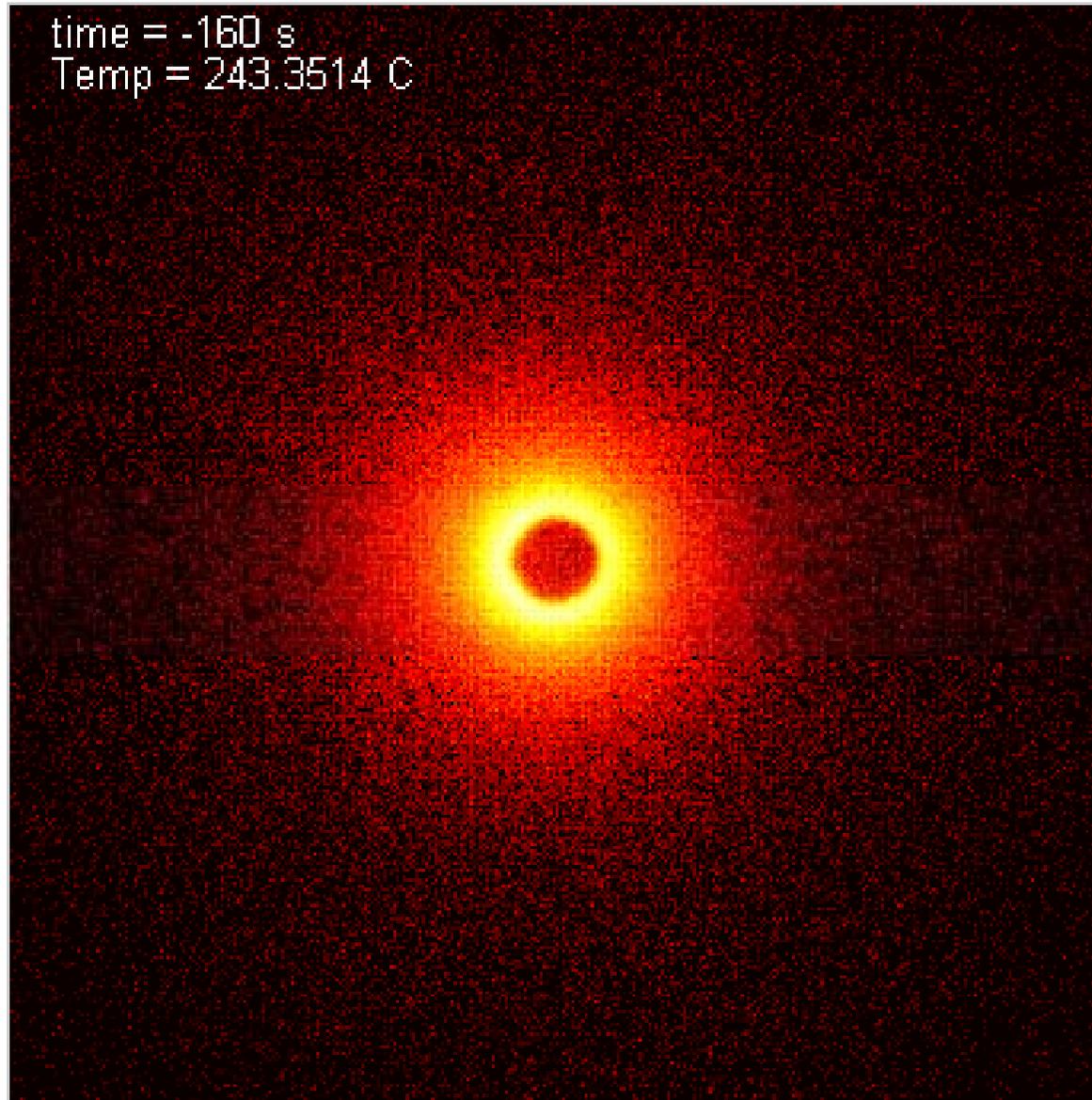
strong orientation



# in-situ Small Angle X-ray Scattering (SAXS)

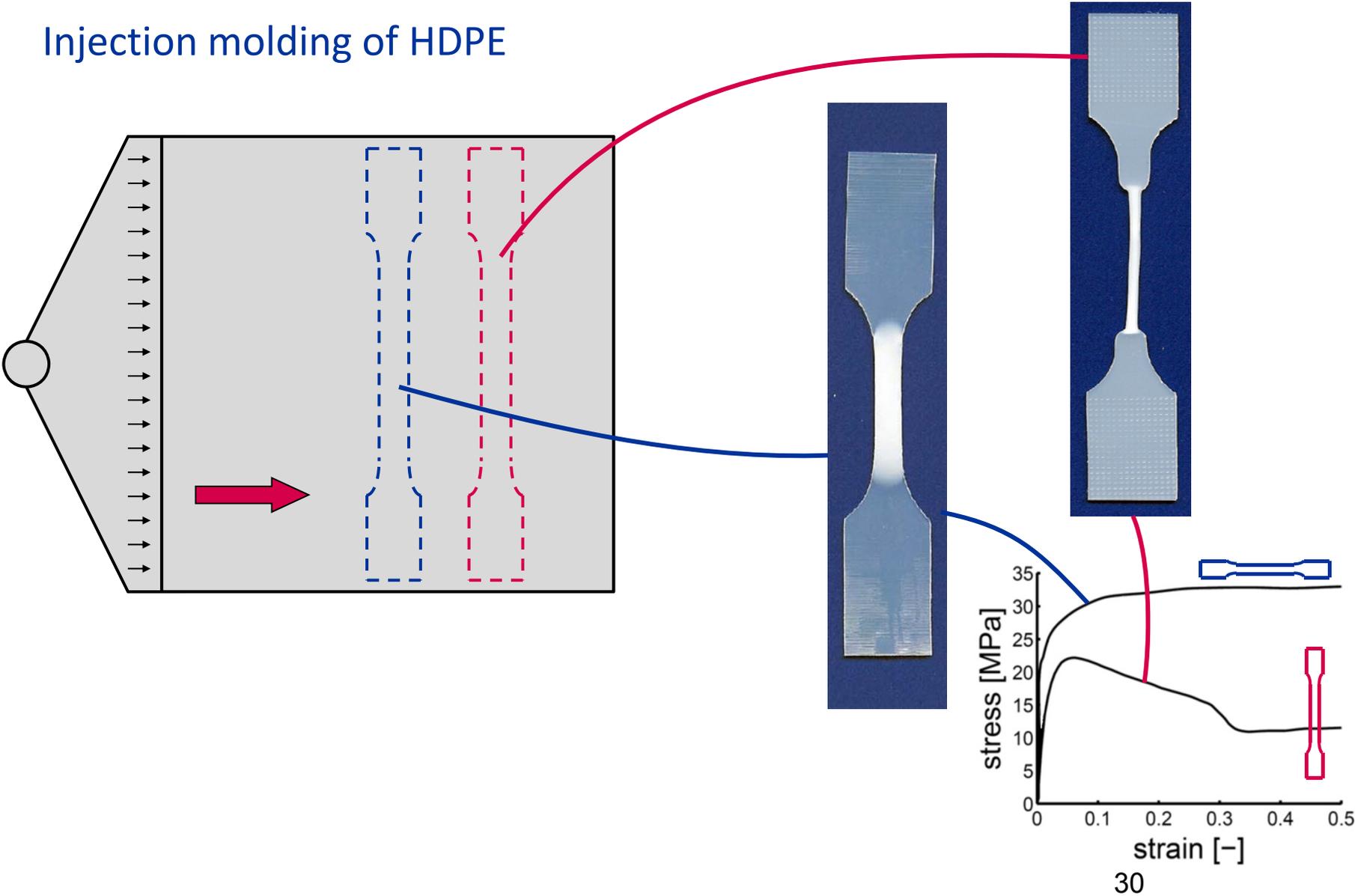


# in-situ: Small Angle X-ray Scattering (SAXS)

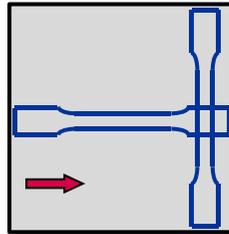


# processing–structure–property

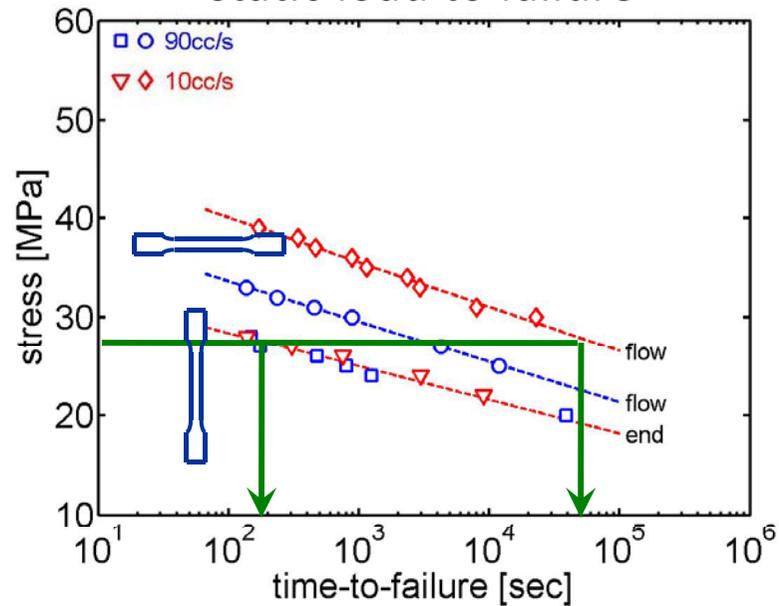
Injection molding of HDPE



# processing–structure–property: example (iPP)

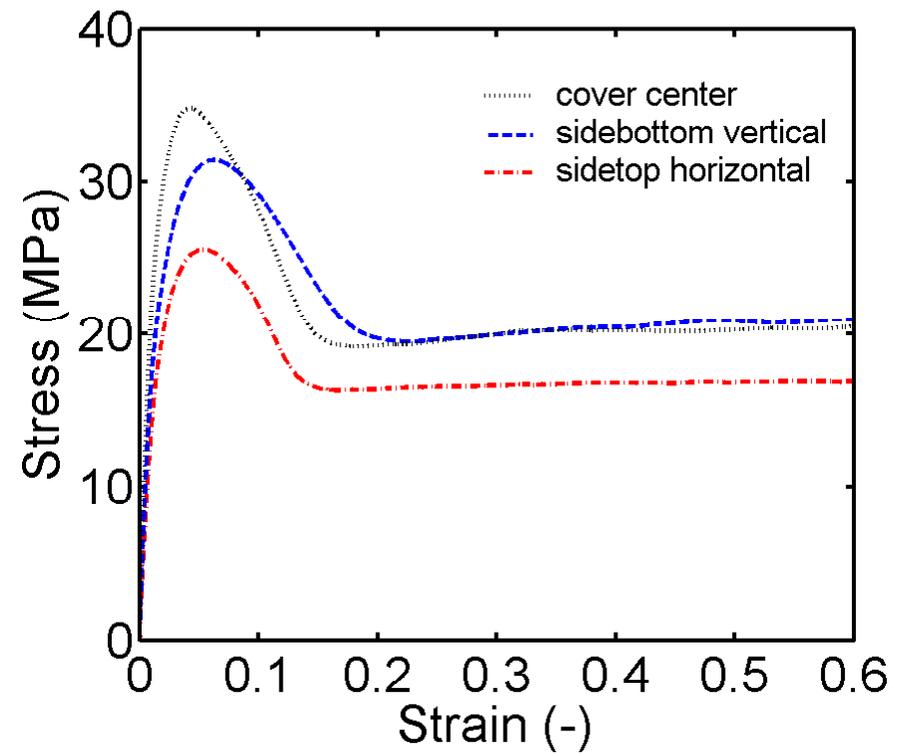


static load to failure

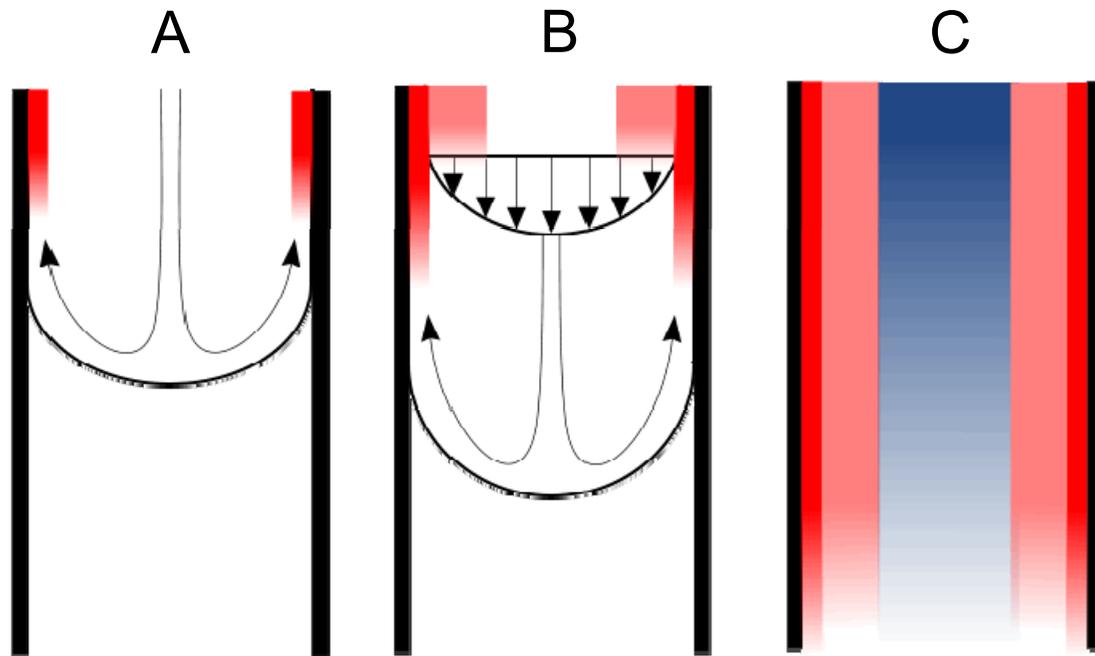


Factor 400 in lifetime for  
different positions/directions!

# processing-structure-properties relations



# processing conditions: injection molding



skin layer

rapid cooling  
( $\sim 100 \text{ }^\circ\text{C s}^{-1}$ )

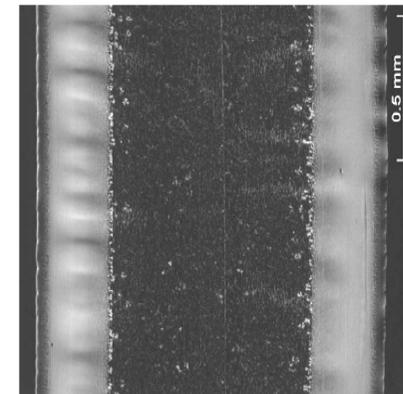
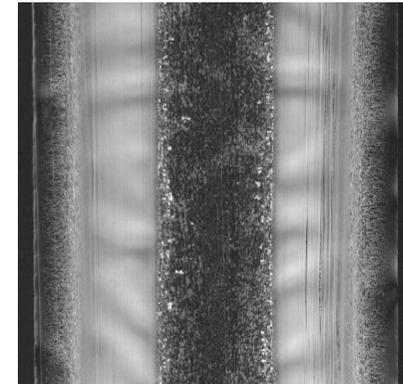
shear layer

flow induced  
crystallization  
( $\sim 1000 \text{ s}^{-1}$ )

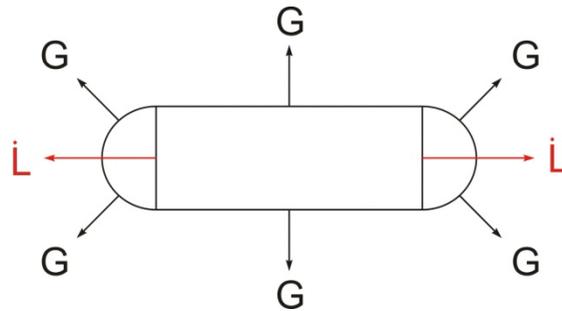
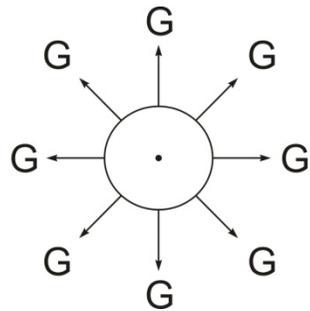
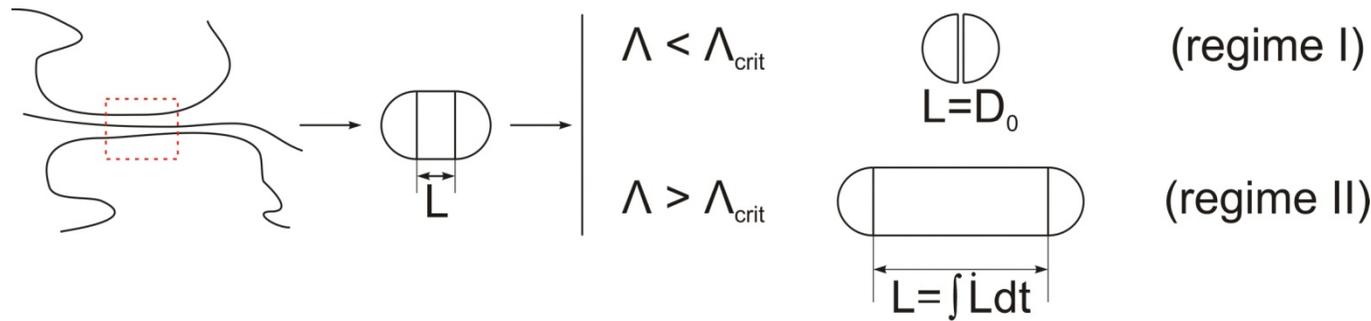
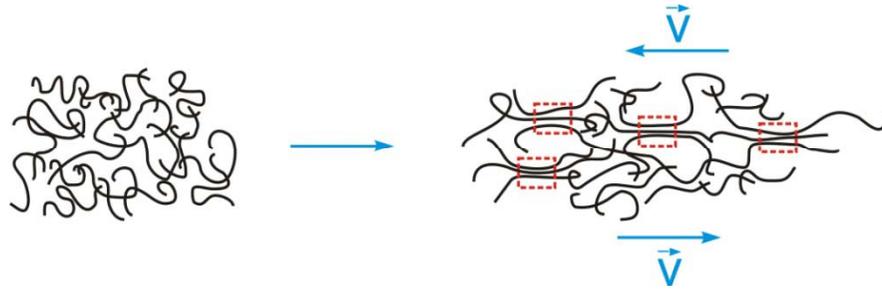
core layer

pressure induced  
crystallization  
( $\sim 1000 \text{ bar}$ )

typical cross section of  
semi-crystalline products



# modeling flow effects on crystallization



# nonlinear viscoelasticity: the eXtended PomPom model

$$\nabla \cdot \boldsymbol{\tau}_i + \boldsymbol{\lambda}(\boldsymbol{\tau}_i)^{-1} \cdot \boldsymbol{\tau}_i - 2G_i \boldsymbol{D} = \mathbf{0}$$

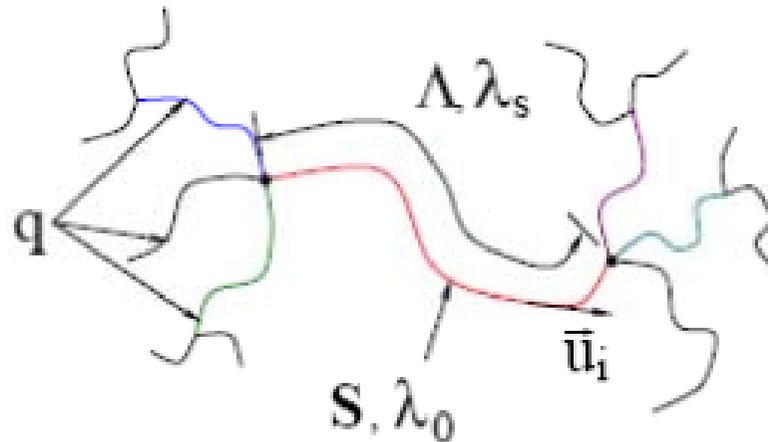
$$\alpha \neq 0 \rightarrow \Psi_2 \neq 0$$

$$\boldsymbol{\lambda}(\boldsymbol{\tau}_i)^{-1} = \frac{1}{\lambda_{b,i}} \left[ \frac{\alpha_i}{G_i} \boldsymbol{\tau}_i + F(\boldsymbol{\tau}_i) \boldsymbol{I} + G_i (F(\boldsymbol{\tau}_i) - 1) \boldsymbol{\tau}_i^{-1} \right]$$

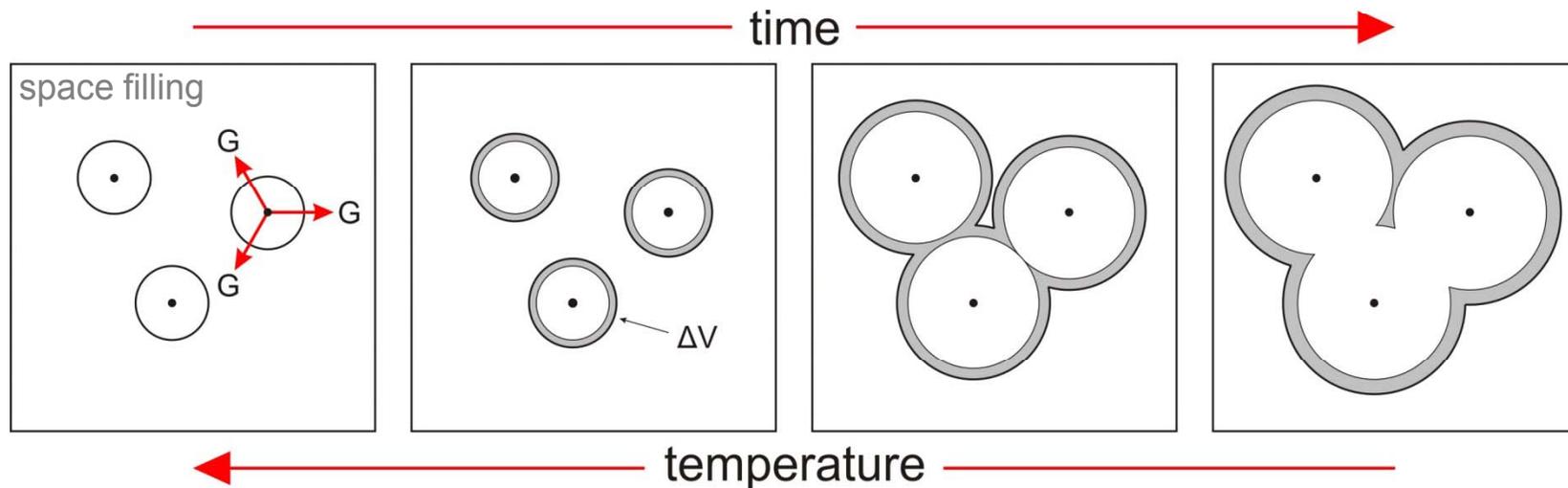
$$\Lambda_i = \sqrt{1 + \frac{\text{tr}(\boldsymbol{\tau}_i)}{3G_i}}$$

$$F(\boldsymbol{\tau}_i) = 2r_i e^{\frac{2}{g_i}(\Lambda_i - 1)} \left( 1 - \frac{1}{\Lambda_i^2} \right) + \frac{1}{\Lambda_i^2} \left[ 1 - \frac{\alpha_i \text{tr}(\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_i)}{3G_i^2} \right]$$

$$r_i = \frac{\lambda_{b,i}}{\lambda_{s,i}}$$



# non-isothermal quiescent crystallization



Schneider rate equations

$$\begin{aligned} \dot{\phi}_3 &= 8\pi\alpha & (\phi_3 &= 8\pi N) & \text{'number'} \\ \dot{\phi}_2 &= G\phi_3 & (\phi_2 &= 4\pi R_{tot}) & \text{'radius'} \\ \dot{\phi}_1 &= G\phi_2 & (\phi_1 &= S_{tot}) & \text{'surface'} \\ \dot{\phi}_0 &= G\phi_1 & (\phi_0 &= V_{tot}) & \text{'undisturbed volume'} \end{aligned}$$

Avrami equation

$$-\ln(1 - \xi) = \phi_0 \quad \text{'real volume'}$$

nucleation density

$$N(T, p) = N_{\max} \exp[-c_N (T - T_{Nref}(p))]$$

individual growth rate

$$G_i(T, p) = G_{\max,i} \exp[-c_{G,i} (T - T_{Gref,i}(p))^2]$$

# flow-induced crystallization

total nucleation density

$$N_{tot} = N_q + N_f$$

(flow-induced) nucleation rate

$$\dot{N}_f = g_n (\Lambda_{hmw}^4 - 1)$$

shish length (L) growth

$$\dot{L} = g_l (\Lambda_{avg}^4 - 1)$$

for  $\Lambda > \Lambda_{crit}$

rate equations

$$\dot{\psi}_2 = 4\pi N_f \dot{L}$$

'length'

$$\dot{\psi}_1 = G\psi_2$$

'surface'

$$\dot{\psi}_0 = G\psi_1$$

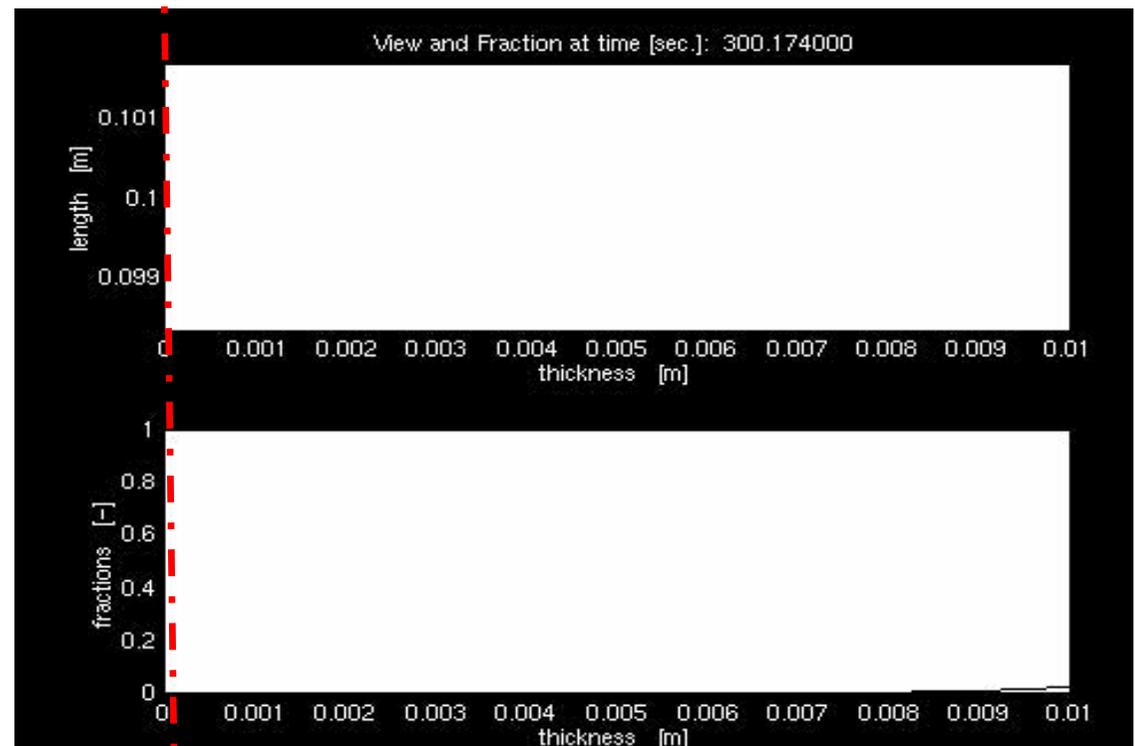
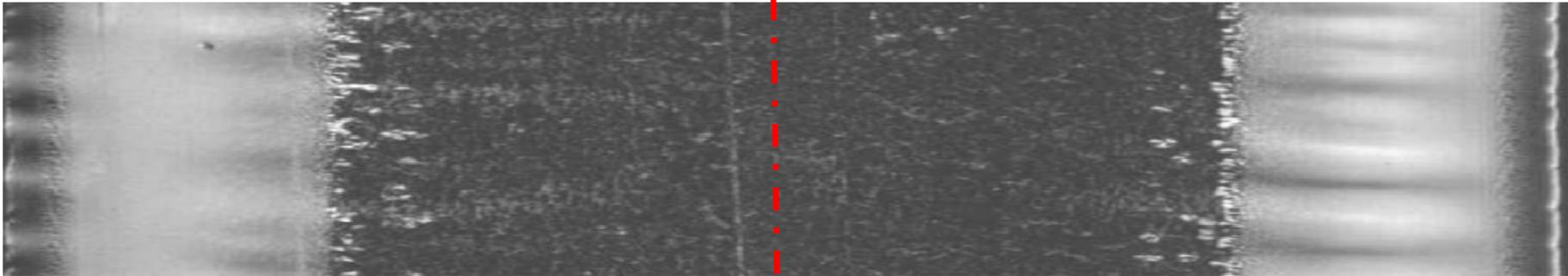
'undisturbed volume'

Avrami equation

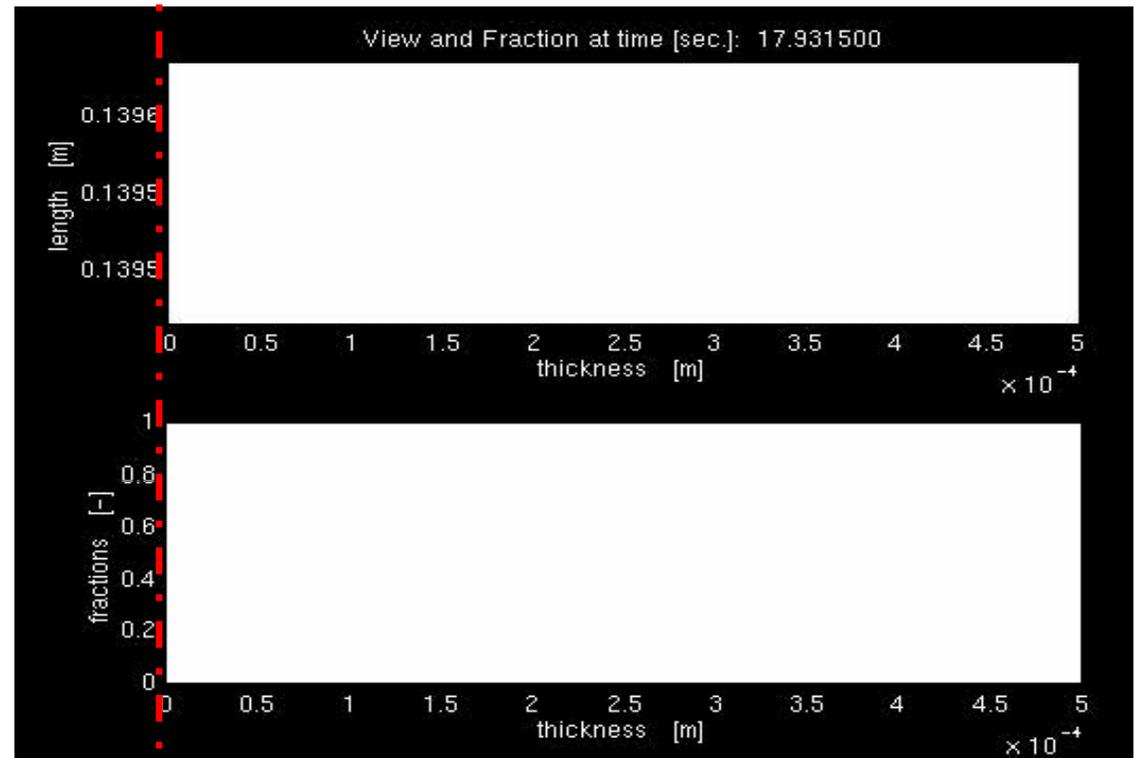
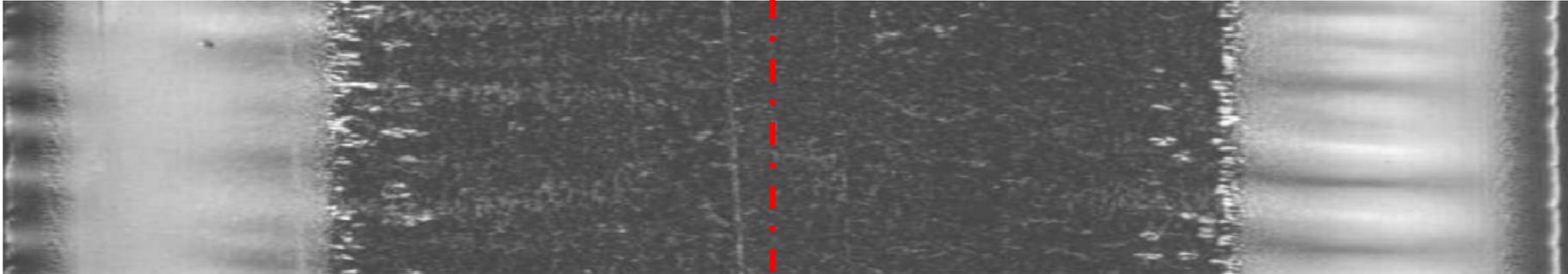
$$-\ln(1 - \xi) = \phi_0 + \psi_0$$

'real volume'

# numerical simulation: no flow

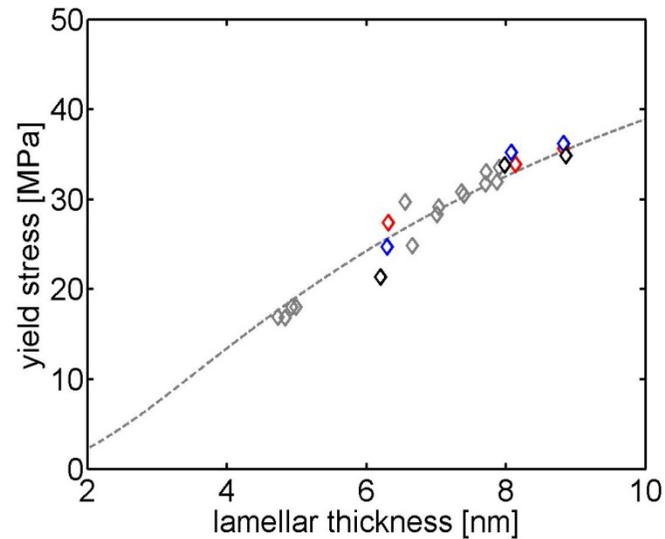
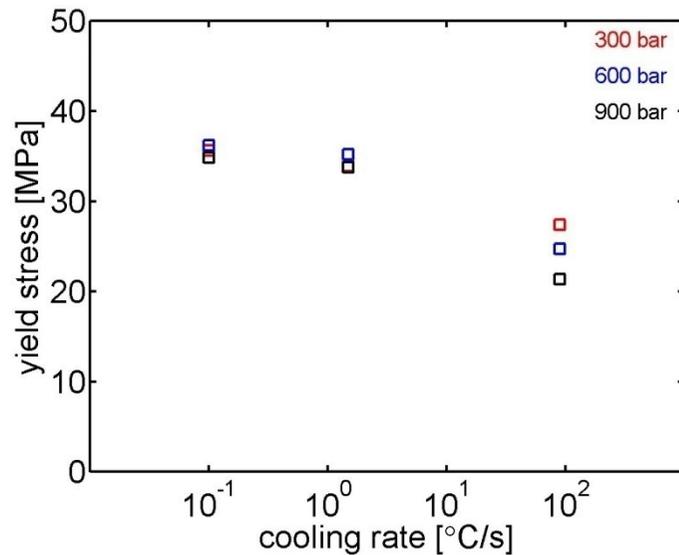


# numerical simulation: flow



# from processing conditions to structure

- use the experimental thermal and pressure history in the model



iPP

so far for the real problems

# acknowledgements



Tim van Erp



Martin van Drongelen



Dario Cavallo



Luigi Balzano



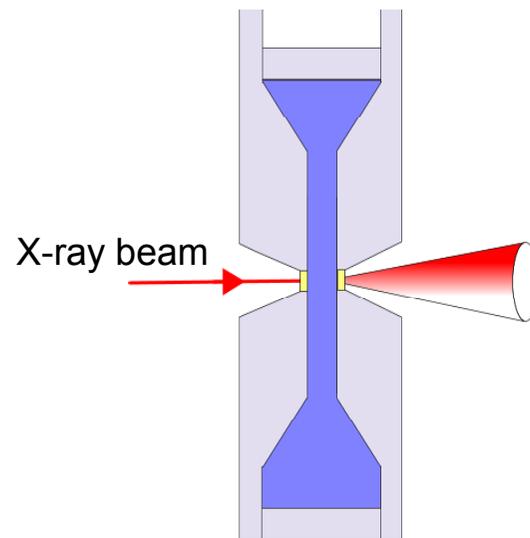
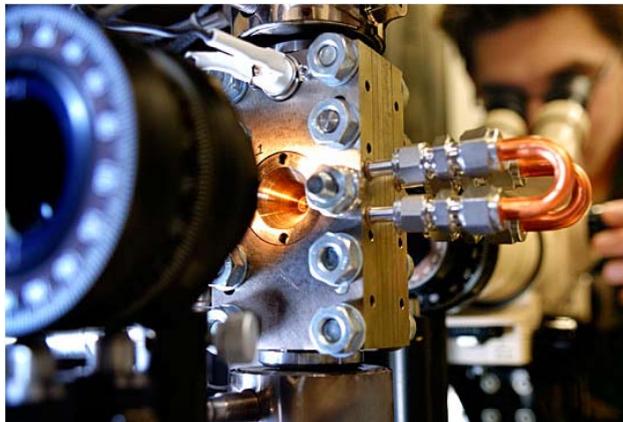
Zhe Ma



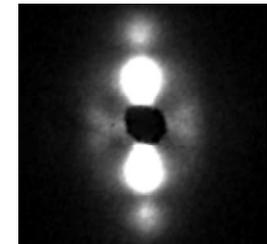
Peter Roozmond



# high pressure, in situ X-ray



SAXS



WAXD

